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6. AUTHOR(S)

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13. ABSTRACT *(Maximum 200 words)*

This grant provided funding for undergraduate and graduate students primarily in support of Grant F49620-93-1-0134 titled "Cluster Ions". A final report for that grant was filed 4/17/96 and contains the primary motivation and accomplishments of the work done. In this report only the work unique to the AASERTS proposal will be listed. This work is primarily involved with investigations of clustering of dihydrogen to transition metal centers and measurement of enthalpies and entropies of attachment using equilibrium methods. We also have begun work on other ligands, such as CH_4, CO, H_2O and cyclopentadienyl (Cp). The focus of this work has been to understand the mechanism of σ-bond activation by transition metal centers through a series of systematic studies using the simplest ligands. These systems can also be subjected to very high level ab initio calculations to aid in extracting the mechanistic information.

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Final Report

AFOSR AASERTS Grant F49620-93-1-305
Carbon Cluster Ions
June 1, 1993 to May 31, 1997

Michael T. Bowers
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Santa Barbara, CA 93106

I. Abstract

This grant provided funding for undergraduate and graduate students primarily in support of Grant F49620-93-1-0134 titled "Cluster Ions". A final report for that grant was filed 4/17/96 and contains the primary motivation and accomplishments of the work done. In this report only the work unique to the AASERTS proposal will be listed. This work is primarily involved with investigations of clustering of dihydrogen to transition metal centers and measurement of enthalpies and entropies of attachment using equilibrium methods. We also have begun work on other ligands, such as CH_4, CO, H_2O and cyclopentadienyl (Cp). The focus of this work has been to understand the mechanism of σ-bond activation by transition metal centers through a series of systematic studies using the simplest ligands. These systems can also be subjected to very high level ab initio calculations to aid in extracting the mechanistic information.

II. Objectives

The original objectives were to characterize structures and formation mechanisms of carbon and metallo carbon clusters. These objectives have been extended to include clustering between transition metal ions and simple ligands.

III. Progress

The primary progress can be found in the various reports for both this grant and the progress reports of the parent grant. They are also presented in detail in the 19 papers published in peer reviewed journals cited in the final report of the parent grant and in the 4 additional papers cited in this report.

The funds provided by this grant were critical for allowing the students freedom to explore new chemistry within the overall framework of the objectives of the grant. Breakthrough experiments and theory were accomplished in the determination of the conformations and folding dynamics of macromolecules in the gas phase, an area of research not felt feasible just a few years ago. This grant specifically supported research that for the first time could allow a detailed look at

the subtle changes in chemistry as either the $4s3d^n$ orbitals of the metal change population moving across the periodic table or in systematic changes in ligands. The key was to generate very accurate data on very simple systems so that experiment and theory could act in concert and extract the key information. Details are given in the papers cited here.

IV. Papers Published or Submitted for Publication*

1. Methane Dehydrogenation by Ti^+: A Cluster Assisted Mechanism for Sigma Bond Activation, P.A.M. van Koppen, J.E. Bushnell, P.R. Kemper and M.T. Bowers, *J. Am. Chem. Soc.* **117**, 2098 (1995).

2. Factors Affecting σ-Bond Activation in Simple Systems: Measurement of Experimental Binding Energies of $Fe^+(H_2)_{1-6}$ Clusters, J.E. Bushnell, P.R. Kemper, and M.T. Bowers, *J. Phys. Chem. Z.* Herman Honor Issue, **99**, 15602 (1995).

3. Details of Potential Energy Surfaces Involving C-C Bond Activation: Reactions of Fe^+, Co^+, and Ni^+ with Acetone, C.J. Carpenter, P.A.M. van Koppen, and M.T. Bowers, *J. Am. Chem. Soc.* **117**, 10976 (1995).

4. Binding Energies of $Ti^+(H_2)_{1-6}$ Clusters: Theory and Experiment, John E. Bushnell, Philippe Mâitre, Paul R. Kemper and Michael T. Bowers, *J. Chem. Phys.* **106**, 10153 (1997).

* Not listed in the final report of the parent grant.

V. Personnel Associated with the Project

Mr. John Bushnell
Ms. Catie Carpenter
Ms. Jennifer Gidden

VI. Papers Presented

A. Invited Lectures at Meetings*

1. Symposium Lecture, Eighth International Symposium on Small Particles and Inorganic Clusters, Copenhagen, Denmark, July, 1996.

2. Symposium Lecture, Molecular Biotechnology Symposium, American Chemical Society Meeting, Orlando, FL, August, 1996.

3. Invited Speaker, Gordon Conference on the Structure, Dynamics and Energetics of Gaseous Ions, Ventura, CA, February, 1997.

4. Plenary Lecturer, New Methods in Ion Cyclotron Resonance, Tallahassee, FL, March, 1997.

5. Symposium Lecturer, Biological Applications of Mass Spectrometry, Pittsburgh Conference, Atlanta, GA, March, 1997.

6. Symposium Lecture, Symposium in Polyethylene Glycol, American Chemical Society Meeting, San Francisco, CA, April, 1997.

7. Symposium Lecture, Fisher Award Symposium, American Chemical Society Meeting, San Francisco, CA, April, 1997.

* Not listed in the final report of the parent grant. These invited lectures were given by M.T. Bowers

B. Contributed Papers by Students

John Bushnell

1. West Coast Ion Chemistry Meeting, Lake Arrowhead, CA, January, 1994 (oral).

2. Gordon Research Conference on the Structure, Energetics and Dynamics of Gaseous Ions, Ventura, CA, February, 1995 (poster).

Catie Carpenter

1. West Coast Ion Chemistry Meeting, Lake Arrowhead, CA, January, 1995 (oral).

2. Gordon Research Conference on the Structure, Energetics and Dynamics of Gaseous Ions, Ventura, CA, February, 1995 (poster).

3. West Coast Ion Chemistry Meeting, Lake Arrowhead, CA, January, 1996 (poster).

Jennifer Gidden

1. West Coast Ion Chemistry Meeting, Lake Arrowhead, CA, January, 1997 (oral).

C. Seminars at Universities*

1. University of Chicago, February, 1996

2. Warwick University (UK), December, 1996

3. Purdue University (two talks), January, 1997

4. Colorado State University, March, 1997

5. University of Colorado at Boulder, March, 1997

6. Michigan State University, March, 1997

7. Northwestern University, March, 1997

8. University of Washington, May, 1997

9. Pacific Northwest National Lab, May, 1997

* Not listed in the final report of the parent grant.